

Freshman Research Initiative Virtual Drug Screening (VDS) Syllabus Spring 2013

Course Uniques:

BIO 206L LAB EXP BIO: STRC/FUNC ORG-FRI	48560
BIO 170C CONFERENCE COURSE-FRI	50715
CH 204 INTRO TO CHEMICAL PRACT-FRI	51635— primary for BlackBoard
CH 108 CONFERENCE COURSE-FRI	52015

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Meeting Times & Class Locations:

Class:
Lab:
Computer Labs:

JGB 2.218, Tues, 3:30 - 4:30pm
PAI 2.14, Times to be determined
WEL 2.144 & ACA 1.126

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Course Overview

This course includes both wet labs and computational/computer-based labs to teach you the skills necessary to find novel drugs against various diseases, pathogens and toxins. The wet lab portion of the course will take place in PAI 2.14. You will be learning basic wet lab techniques that are important in a research environment as well as specific techniques for our research. By the end of the semester you will be competent in preparing solutions, spectrophotometry, titration using pH, and protein expression, purification and characterization of purity and yield. On the virtual side, you will be able to analyze 3 dimensional structures of macromolecules, interface remotely with a High Performance cluster computer to carry out computational screening, and assess small molecule binding to a target based upon the output of a molecular docking program.

Computer labs will initially be spent learning how to visualize and analyze protein structures and protein-ligand interactions through the program PyMol (<http://www.pymol.org/>). PyMol is available on the computers in the Welch Hall Computer Lab (WEL 2.144). You are encouraged to install the free version (Release 0.99 pymol-0_99rc6-bin-win32.zip under 'Legacy' at <http://sourceforge.net/projects/pymol/files/>) on your own computer and become familiar with the use of the program. Instructions on the use of PyMol form the basis of the first three computer labs while molecular docking programs will be used in the later labs to carry out virtual screening. Lab time will be scheduled in WEL 2.144 and/or ACA 1.126, but some of the work can be performed independently.

Spring 2013 Experiment Schedule:

Wk	Start Date (Tues)	Experiment	Assignment
1	1/15 - Tues	Introduction, Lit Assignment, Bibliography Assignment, Lab tours and lab safety walk throughs	Lit Assign, EndNote Assign, and Lab Safety due 1/21 (Mon) at midnight (m/n)
2	1/22	Lab: Buffer & Solutions (No lab report – only notebook) -- Start your Mini Research write up	<u>Lab Notebook</u> due 1/26 (Sat at 5 pm)
3	1/29	Lab: Pymol lab 1 -- Continue Mini Research write up	Mini Res Write up due 2/4 (Mon at midnight)
4	2/5	Lab: Beer's Law	<u>Lab Notebook</u> due 2/9 (Sat at 5 pm) Beer's Law Lab report due 2/11 (Mon at m/n)
5	2/12	Lab: Pymol lab 2	Peer review for Beer's Law Report due 2/18 (Mon at m/n) Wiki Posting due 2/18 (Mon at m/n)
6	2/19	Lab: Buffer Titration	<u>Lab Notebook</u> due 2/23 (Sat at 5 pm) Final Version of Beer's Law Report due 2/25 (Mon at m/n)
7	2/26	Lab: Pymol lab 3	
8	3/5	Lab: Bacterial protein expression (start mon)	Combined Lab Report with other protein labs (4/15) <u>Lab Notebook</u> due 3/8 (Fri at 9 pm)
9	3/12	No lab (spring break)	
10	3/19	Lab: Virtual Screening 1	Lab report due 3/25 (Mon at m/n)
11	3/26	Lab: Protein purification	Combined Lab Report with other protein labs (4/15) <u>Lab Notebook</u> due 3/30 (Sat at 5 pm)
12	4/2	Lab: Virtual Screening 2	
13	4/9	Lab: Protein characterization	Combined Lab Report with other protein labs due 4/15 (Mon at m/n) <u>Lab Notebook</u> due 4/13 (Sat at 5 pm)
14	4/16	Lab: Virtual Screening 3 & Enzyme Assay Target Discovery Exercise	
15	4/23	Lab: Virtual Screening 3 & Enzyme Assay	
16	4/30	Class and Lab Cleanup	Final Lab report due 5/2 (Thurs) <u>Lab Notebook</u> due 5/2 (Thurs at 7 pm)

Quantitative Reasoning Flag:

This course carries the Quantitative Reasoning flag. Quantitative Reasoning courses are designed to equip you with skills that are necessary for understanding the types of quantitative arguments you will regularly encounter in your adult and professional life. You should therefore expect a substantial portion of your grade to come from your use of quantitative skills to analyze real-world problems.

<http://www.utexas.edu/ugs/ccc/flags/quantitative-reasoning>

Meeting Times:

The weekly class meetings are mandatory. The lecture portion will provide the theoretical background for the lab and helpful hints and details on how to perform the experiments, proper use of equipment, and data interpretation. You are expected to take notes during the class since most of the material is not contained in a textbook or the handouts.

The times in lab are also mandatory but the time will vary based upon the given experiment. If you cannot make a class meeting or the lab, then you need to contact the RE in advance.

You are required to **sign in** when you come to lab so that we have a record of your work (in binder near door). You are also required to have a mentor, TA, or RE check you out each time you leave the lab. This is to verify that you have left your lab space clean, which counts towards your Lab Conduct grade.

Office Hours:

You can always make appointments with the RE for help and discussion outside of the allotted lab times. The mentors and the TA may be contacted via e-mail with quick questions outside of lab but they are not obligated to spend extensive time in this manner. Consequently, you may be referred to the RE.

Course Communication:

- Announcements, course handouts and protocols will be available via handouts, email or posted on Blackboard. <http://courses.utexas.edu> and/or on [Google Docs](#). You are expected to check your email and BlackBoard on a regular (daily basis) for any pertinent course communication. Class slides will be posted to online a few days after each class.
- Face to face, email, text and phone are all acceptable methods of contacting the RE.
- A wiki/blog page will be used as part of the Mini Research Assignment to share information amongst the class about the various targets. (Wikispaces)
 - **NOTE:** When you create an account for Wikispaces, use your first name and last initial for the login. e.g. joshb. If you have the same first name and last initial as someone else - then the next letter in your last name e.g. joshbe

Scheduling:

We will keep track of scheduling in the labs by using Google calendar. For the Painter lab, we will use the calendar to show when mentors, the TA or the RE will be present. We may also use it to reserve certain pieces of equipment (e.g. PCR machines, spectrophotometers) if it gets too crowded.

Google Calendar for the VDS class

Login: **vdsclass@gmail.com**

Password:

The Painter lab should be open from 9 AM to 9 PM every weekday. There will also be some hours on Saturday and/or Sunday which are yet to be determined.

You can only work in the lab if a **mentor** or **TA** or **RE** is present! This is for safety reasons.

Course Assessment

Since this course is not a typical Lab course, the course will also be evaluated on a different basis. You will learn that in research, experiments don't always work. Sometimes you might follow the protocol but still not get expected results. Science is a process of trial and error, as long as you learn from your failure it is a success. You are expected to understand the theoretical background of the techniques you are using and to keep a good record of what was done in the Lab. This will be recorded in your Lab notebook and summarized in a weekly Lab report for evaluation.

Course Weighting:

Lab notebook	30%
Lit. Search Assign. + Bibliography	3%
Mini Research Write up + Wiki Page	8%
Lab reports	30%
Quizzes and misc. assignments	11%
Final Lab report	12%
Lab Conduct/effort + Lab Safety	6%
Total	100%

NOTE: Late assignments will lose **5%** of their total value per day

Plus/minus Grading:

The Virtual Drug Screening stream will take advantage of the plus/minus grading system for your final grade in the class, wherein:

A = 4.0, A- = 3.67, B+ = 3.33, B = 3.0, B- = 2.67, C+ = 2.33
C = 2.0, C- = 1.67, D+ = 1.33, D = 1.0, D- = 0.67, F = 0.0

However, assignments during the course will be graded on a 10 point system, which will then be weighted by assignment and converted to the 4 point system at the end of the semester to calculate your final grade:

(10, 9.75, 9.5, 9.25, 9.0, 8.75, 8.5, 8.25, 8.0, 7.75, etc..) .

Grades may be curved at the end of the semester. You will be assessed on your abilities and effort amongst your classmates and upon your progress through the semester. An 'A' represents exemplary work beyond merely what has been assigned, an 'A-' represents completing everything that is asked in the class and understanding of the material, a 'B+' is for those that have missing or late assignments or are deficient in their understanding. 'B' is for those that have missing or late assignment and are deficient in understanding. Lower grades represent further degrees of the above.

Lab Reports:

Reports are to be handed in or electronically submitted before our weekly class meetings unless otherwise notified. In addition, a **Final Lab report** that incorporates the last 2 labs will be due at the end of the semester. These reports will help you develop technical writing skills. Comments will be given and you will be graded on how your writing improves over the semester. Some reports will be combined and will count for their summed value of points.

Any work that is to be submitted electronically (via email or upload to BlackBoard or GoogleDocs) should have a descriptive filename so that it can be sorted easily. For example, name your file with

UTEID_Name_Date_AssignmentName.pdf

e.g. REF289_RosalindFranklin_Jan232013_Assignment1BuffersLab.pdf

NOTE: your **name**, **document title** and **page numbers** must be in the 'header' or 'footer' for all work submitted electronically. This is necessary so that when I print them out to write comments – I will know which pages belong to you! See the bottom of this page for an example.

e.g. "Rosalind Franklin Buffers & Solutions Lab

p. 3"

Lab Notebooks:

The detail and clarity of your notebook will be very important in conveying your understanding and effort. A lab notebook grading rubric will be provided which will allow you to see exactly what needs to be included. The notebook needs to be updated continuously as you perform experiments.

- You are required to write EVERYTHING pertaining to experiments in the lab notebook
- Graphs, spreadsheet data and images should be pasted into the lab notebook when appropriate
- Sketches and diagrams are encouraged!

Try to keep a sequential flow to the notebook, but when this is not possible then it is necessary to place page numbers so that you can refer to where an experiment picks up again. The RE will schedule lab notebook checks and randomly examine the individual notebooks through the semester as there is seldom a time to collectively evaluate them together.

- Lab notebooks must stay in the lab. You will not be allowed to take them home with you. So, plan to arrive early to start filling out your notebook before lab and then, if necessary, you can come in after your lab on another day to finish it up.
- Since the notebooks are property of the lab, they will be left with the stream at the end of the semester. It is your responsibility to make duplicates of protocols and data you wish to keep. Also, when you are writing your lab reports – you may want access to some of the information in your notebook. The best way to do this is to take pictures of your lab notebook pages beforehand.
- The wet lab entries must be handwritten, but computer labs (PyMol and Virtual Screening) can be pasted in from a WORD document that you will have created while in the computer lab (your work and modifications to protocol should be type in green/blue font). **Diagrams** and **sketches** are encouraged in your labnotebook – ‘a picture is worth a thousand words’

We require buying a lab notebook that is sturdy, can be written on both sides, large enough to paste graphs and figures into, and small enough to store easily in a drawer and not take up too much bench space when you are working in the lab

- Blueline notebooks (A9Q or A9, with or without grids, 192 pages costs \$5.95) from the COOP

The large carbon copy notebooks for some of the other chemistry course are NOT allowed – due to their size. Also, the ‘composition’ notebooks common for humanities classes are not permitted – they are too flimsy.

Lab Conduct/Effort:

You will be evaluated on a few basic principals of lab conduct that all good researchers (and workers in general) should possess:

1. **Enthusiasm:** How much desire the student has to learn the topics and apply them.
2. **Initiative:** How often a student proceeds independently on an experiment.
3. **Follow-through:** How well the student can complete an experiment correctly in a timely manner, once asked to.
4. **Absorptiveness:** How well the student understands the methods and can interpret data.
5. **Synthesis:** How well the student can develop new ideas and implement methods to new problems, design relevant experiments, and test those ideas.
6. **Writing/Organizational Ability:** How well the student can keep notebooks, explain or present ideas, describe the data and its meanings (reports), manage time, and express themselves.
7. **Cleanliness:** How well the student prevents contamination and cleans up after themselves. This will be evident in the experimental results and bench area. Be a good lab citizen.
8. **Collaboration:** How well the student collaborates with peers and communicates ideas effectively. This includes accurate descriptions of figures and the procedures they have done.

Please respect the equipment and keep it in good working order. You are expected to keep the area clean where you have carried out your experiments since this space is shared with three other VDS streams. Your lab grade will be partially dependent upon how well you cleanup after working in the lab and keeping the VDS supplies and reagents organized. A good habit to get in, is to try and clean at least one thing that is not yours

before leaving the lab. This may simply be throwing away a loose tube on the floor or washing a piece of glassware. As you begin to work in smaller labs, your responsibility will increase and your cooperation will be appreciated even more by other lab members.

Organization

Materials:

Tubes, plates, boxes, vials, bottles, and etc. must always be labeled appropriately or it will be discarded. In most cases you will use a short piece of colored tape to make a label. A complete label has the following information: VDS, Your Name (or initials), Date, Contents, Concentration, Experiment or sample number. All items should be labeled in 2 places: on the top and side. This is for redundancy for when one of the labels falls off or the ink is removed by a solvent.

Ice (not for human consumption) and autoclaves can be found in PAI 1.03. You are allowed to get ice on your own but autoclaving will be done by the mentors, TA or RE. Do not wear gloves in the hallway or outside the building.

Computers:

This course requires the use of computers for data collection, data analysis, and for communication purposes. We expect you to use your own data backup methods (UT Webspaces: <http://webspace.utexas.edu/>, Gdrive, DropBox, or a thumb drive) to store all computer files generated. Some of the lab computers are re-imaged and are not a reliable place to store your files. It is your responsibility to have a back up of your data. PAI 2.14 has wireless access. Computer labs are available nearby in WEL 2.144 and ACA 1.126

Lab Safety Training

The following courses are required to be completed by the students enrolled in the Virtual Drug Screening stream. There is usually a short quiz that you must complete after each course. A copy of your training record must be printed out and submitted to the Research Educator (Dr. Beckham). The training record can be seen in TxClass by clicking on the 'Training History' link. This must be done before the first wet lab (Beer's Law) in PAI 2.14 (Painter Hall) is started.

DUE DATE: Monday January 21st at Midnight – bring printout to class or lab

General Info: Environmental Health and Safety Site for general information:

<http://www.utexas.edu/safety/ehs>

This course should have been completed by you in the fall Research Methods class– if not, do now:

OH 101 General Hazard Communication - online

<http://www.utexas.edu/safety/ehs/train/courses.html#oh101/>

These are the ones to be taken for Spring:

OH 102 Site Specific Hazard Communication - in person

To be completed in first week with Research Educator in the Painter 2.14 Lab.

This course may not show up in your Personal Training History for a week or so

OH 201 Laboratory Safety – online

<http://www.utexas.edu/safety/ehs/train/courses.html#oh201>

OH 202 Hazardous Waste Management – online

<http://www.utexas.edu/safety/ehs/train/courses.html#oh202>

We will also need recombinant DNA training (**CW512**) through the IBC

https://utdirect.utexas.edu/cts/class.WBX?s_course_comp=0&s_course_prefix=CW&s_course_number=0512

Verify your completion through Personal Training History:

<https://utdirect.utexas.edu/txclass/> (go to 'Training History')

Safety & Waste Disposal

We may handle organic solvents (some may be highly corrosive to human skin and tissues) and other potentially dangerous chemicals and items. Safe lab practices and waste disposal procedures are mandatory and will be taught to you. Unsafe, imprudent and careless activities will result in you being removed from the lab. Continued

noncompliance will result in a reduced lab grade and/or course failure. Please report anything you see that is unsafe (confidentially) to the TA or mentors.

1. Know the nearest location and proper use of the fire extinguisher (by both doors), first-aid kit and chemical spill-kit (both under the nanopure), eye-wash (middle sink).
2. Students must be supervised at all times while working in the laboratory.
3. Immediately report any accidents or mishaps to the mentors, TA, or RE.
4. You are required to wear latex or nitrile gloves when performing experiments. Know when to use latex vs nitrile. Also, know the location of safety glasses (cabinet) and lab coats (hanging on closet door next to entrance). Wear these safety items at all times especially when working with hazardous chemicals.
5. Always wear closed toed shoes and pants (NO SANDALS or SHORTS). Otherwise, you will have to wear booties and a lab coat or go home to change. You are welcome to keep a pair of clothes in a cubby to change into.
6. No food or beverages are allowed in the laboratory. PERIOD.
7. DO NOT store book bags on lab benches. They may go in the cabinets under the desks.
8. For your own safety and that of others, discard all waste appropriately:
 - a. Razor blades, needles, and other sharp METAL items should be placed in the Red plastic SHARPS containers
 - b. Glass must be placed in white cardboard boxes labeled "For Glass Disposal".
 - c. Certain chemicals (PAGE and Phenol/Chloroform) must be placed in labeled waste containers in the chemicals hood.
 - d. Biologicals (bacteria) like LB agar plates must be placed in orange Biohazard waste containers for autoclaving. Liquid cultures must be killed with 10% bleach for 20 minutes and disposed down the center sink drain.
9. Glassware is to be washed promptly after use.
 - a. Remove ink or tape labels with ethanol or Goo-B-Gone.
 - b. Scrub items with sponge or bottle brush and warm soapy water (Alconox – powder)
 - c. Triple rinse with tap water until soap is gone.
 - d. Inspect for cleanliness. If not clean, wash again.
 - e. Double rinse with distilled tap water.
 - f. Drain excess water in sink.
 - g. Invert all items to dry on peg boards or other designated locations for next class. Note, drying racks are provided for items that are easily tipped over. Once dry, replace to glassware cabinet.
10. The lab room should be as clean (or cleaner) when you leave, as it was when you arrived.
11. Report any problems or mishaps to your RE.

During certain laboratory exercises, you may be given special instructions regarding disposal of hazardous materials, chemical solutions such as organic solvent wastes, or biological material such as antibiotic-resistant bacteria. For your own safety and that of others, please follow these special directions carefully

ALWAYS ASK QUESTIONS BEFORE YOU DO SOMETHING IF YOU ARE UNSURE!

Accommodations

Please notify your instructors at the beginning of the semester of any modification/adaptation you may require to accommodate a disability-related-need. You will be requested to provide documentation to the Dean of Students' Office, in order that the most appropriate accommodations can be determined. Specialized services are available on campus through Services for Students with Disabilities (471-6259).

Appeals

The Research Educator, TA and Mentors will make decisions concerning grades, attendance and other policy matters. Should you disagree with a TA or Mentor, you are welcome to take the matter to the RE.

Academic Integrity

Policies for academic dishonesty are designed to help you and to be fair to the other individuals in the class. Scholastic dishonesty will not be tolerated. Being honest about your academic work is the foundation of your education. For this reason, cases of academic dishonesty will be regarded with the utmost seriousness whether this means copying someone else's Lab report or making up lab results. If quoting or paraphrasing from another source, please ask instructors, TA or mentors on the correct way to cite a reference. For a complete definition of unacceptable behavior, such as plagiarism, and the UT policy regarding such activities, see the Student Judicial Services website: http://deanofstudents.utexas.edu/sjs/acint_student.php.